

# ***First Workshop on Predictive Capabilities for Strongly Correlated Systems***

Sponsored by the US Department of Energy and The University of Tennessee

**The University of Tennessee, Knoxville**

**November 7-9, 2003**

---

**Friday, November 7**

555 Buehler Hall (Chemistry Building)

**Chair: Warren Pickett**

- 16:00 – 16:40    **Vladimir Antropov**, Ames National Laboratory  
*Microscopic theory of magnetism: Current status and problems*
- 16:40 – 17:20    **Mark Jarrell**, University of Cincinnati  
*Combining quantum Monte Carlo and perturbation theory*
- 17:20 – 17:35    **Chris Marianetti**, Massachusetts Institute of Technology  
*Electronic correlations in  $\text{Li}_x\text{CoO}_2$*
- 17:35 – 17:50    **Kwan-Woo Lee**, University of California, Davis  
*Charge- and spin-ordering tendencies in  $\text{Na}_x\text{CoO}_2$*

---

17:50 – 18:20 Coffee Break

---

307 Science and Engineering Building

**Chair: Cyrus Umrigar**

- 18:20 – 19:00    **James Gubernatis**, Los Alamos National Laboratory  
*New mechanisms for itinerant ferromagnetism and electronic ferroelectricity: The joys and challenges of mixed valency*
- 19:00 – 19:15    **Thomas Maier**, Oak Ridge National Laboratory  
*On the nature of pairing in the cuprates*
- 19:15 – 19:30    **Ping Sun**, Rutgers University  
*Comparison of approximation schemes for many-body systems*
- 19:30 – 19:45    **Ramiro Pino**, Rice University  
*Laplace-transformed diagonal Dyson correction to quasiparticle energies*

19:45–20:00     **Alexandru Macridin**, University of Cincinnati  
*Electron-hole asymmetry in cuprates and the validity of the one-band Hubbard model*

---

Dinner on the Cumberland Strip/Hotel/Calhoun's by the River/Tennessee Grill (on your own).

---

### Saturday, November 8

307 Science and Engineering Building

**Chair: John Wilkins**

8:30 – 8:45     **Billie Collier**, Associate Vice President for Research, UT  
                  **Richard Scalettar**, UC Davis-**Adolfo Eguiluz**, The University of Tennessee

8:45 – 9:00     **Dale Koelling**, Department of Energy  
                  *Welcome to the Computational Materials Science Network*

9:00 – 9:40     **Ole K. Andersen**, Max-Planck Institut, Stuttgart  
                  *Wannier-like functions from downfolding. Low-energy Hamiltonians for transition-metal oxides*

9:40 – 10:20    **Jörg Fink**, Leibniz Institut für Festkörper und Werkstoffforschung, Dresden  
                  *Electronic structure studies of undoped and doped cuprates using high-energy spectroscopies*

10:20 – 10:40   **Claude Ederer**, University of California, Santa Barbara  
                  *Spin and orbital moments in Fe and Co systems with various dimensionalities*

---

10:40 – 11:10 Coffee Break

---

**Chair: Shiwei Zhang**

11:10 – 11:50   **John Perdew**, Tulane University  
                  *Climbing Jacob's Ladder: The Meta-GGA for exchange and correlation*

11:50 – 12:30   **Steve White**, University of California, Irvine  
                  *Renormalization group methods for electronic structure*

12:30 – 12:50   **Ward Plummer**, The University of Tennessee  
                  *A novel surface Mott-insulator transition in the layered ruthenate  $\text{Ca}_{1.9}\text{Sr}_{0.1}\text{RuO}_4$*

---

12:50 – 14:00 Lunch Break                    (201 Physics Bldg.)

---

---

**Chair: Richard Scalettar**

- 14:00 – 14:40     **Jonathan Denlinger**, Lawrence Berkeley National Laboratory  
*Strong motivations from ARPES for realistic correlated-electron theory:  $V_2O_3$ , hexaborides and other challenges*
- 14:40 – 15:20     **Henry Krakauer**, College of William and Mary  
*Quantum Monte Carlo method for real materials: Phase-free random walks in Slater-determinant space*
- 15:20 – 16:00     **Mark van Schilfgaarde**, Arizona State University  
*Self-consistent GW method*

---

16:00-16:30    Coffee Break

---

**16:30-18:30       PCSCS talks (six funded projects) and discussion**

**19:30 – 22:00 Workshop Dinner — Knoxville Convention Center (KCC)**

**22:00 – 23:00 Informal Networking, at 301 KCC**

---

**Sunday, November 9**

307 Science and Engineering Building

**Chair: Adolfo Eguiluz**

- 9:00 – 9:40        **Gabriel Kotliar**, Rutgers University  
*First-principles electronic structure calculations of correlated materials using dynamical mean field theory*
- 9:40 – 10:20      **Zahid Hasan**, Princeton University  
*Inelastic x-ray scattering as a probe of correlated electrons: Current status and future directions*
- 10:20 – 11:00     **Mark Lumsden**, Oak Ridge National Laboratory  
*Neutron scattering in strongly correlated electron systems*

---

11:00 – 11:30 Coffee Break

---

**Chair: Thomas Schulthess**

- 11:30 – 12:10     **Richard Martin**, Los Alamos National Laboratory  
*An overview of hybrid DFT applied to metal oxides*

- 12:10 – 12:50    **Wei Ku**, Brookhaven National Laboratory  
*Simple construction of energy-resolved Wannier states with assigned local symmetry; Application to quasi-1D Cu-O spin chains*
- 12:50 – 13:10    **Richard Hennig**, The Ohio State University  
*Correlated phase transitions on the atomic length scale: The mechanism for the Ti hcp to omega martensitic transition and how impurities block the transformation*
- 13:10 – 13:30    **Trevor Tyson**, New Jersey Institute of Technology  
*Structural, magnetic and spectroscopic studies of thin manganite films*
- 13:30 – 13:50    **Todor Mishonov**, University of Sofia  
*3d-to-4s-by-2p highway to superconductivity in overdoped cuprates*
- 13:50 – 14:00    **Closing Remarks; Warren Pickett, UC Davis**

---

14:00    Lunch Break                      (201 Physics Bldg.)

**14:30-16:30        PCSCS Networking                      (201 Physics Bldg/ 307 S&E)**